T-4
Atomic & Optical Theory

LANL T-4 Opacity Web Page

Norman H. Magee, Jr. (T-4) and Robert E. H. Clark (X-CI)

Introduction:
Group T-4 of the Theoretical Division has been involved in calculating opacities since the 1970s. Many mechanisms have been employed over the years to distribute and display this large data base (more than 10 gigabytes) to users both within the Laboratory and around the world. We have now combined the data base with a fast data handling code, a graphics package and the World Wide Web (WWW) to provide users with greatly expanded flexibility to access, view and obtain a wide range of opacity calculations.

The Data Base:
The Astrophysical Opacity data base contains opacity information for all elements from hydrogen to zinc, over a temperature range from 0.5 eV to 100 keV and a density range from 10^{-10} to 10^{+9} gm/cc. Every element has approximately 1500 (T-η) points, where T is the temperature and η is the electron degeneracy parameter, which characterizes the electron pressure of the plasma at the ion-plasma boundary. Each (T-η) point has 14,900 frequency-dependent opacity values on a common u grid ($u = h\nu /kT$), as well as integrated opacities (Rosseland and Planck) and the average stage of ionization.

The Astrophysical Opacity data base contains opacity information for all elements from hydrogen to zinc....

The Los Alamos Light Element Detailed Configuration OPacity (LEDCOP) code calculates the opacities in local thermodynamic equilibrium (LTE). It uses the Saha equation, including degeneracy, where the Rydberg sequences are cut off by plasma interactions. Each ion stage is considered in detail, using an LS basis set calculated by a self-consistent Hartree-Fock code. Nonhydrogenic oscillator strengths and photoionization cross sections are also calculated and incorporated into the calculations. Interested readers should access the web page reference link for more details.

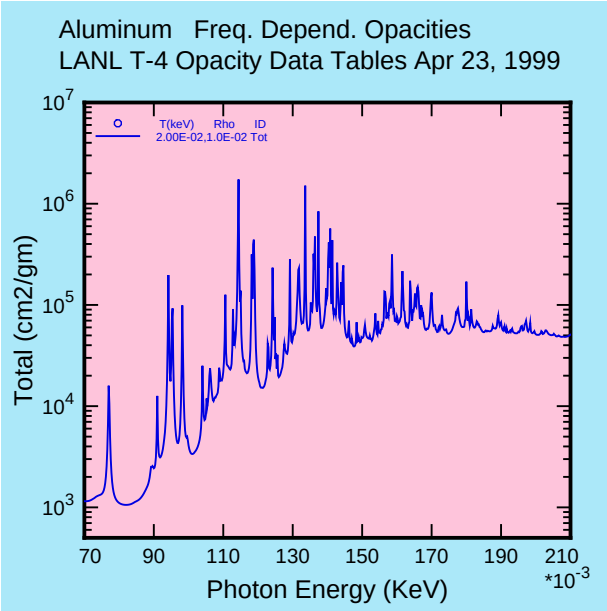

Figure 1: Plot of the total (absorption and scattering) frequency-dependent opacities for aluminum at a temperature of 0.02 keV and a density of 0.01 gm/cc. Printed from the 2D frequency-dependent opacity option.

Data Handling and Graphics Codes:
The data base consists of random access binary files which are read and manipulated by the TOPS multigroup opacity code. Since all of the elements are on uniform T, η , and u grids, this code can take the individual element data and mix them together to calculate an opacity table for any desired material. This table can

then be interpolated in density (temperatures can not be interpolated) to obtain the opacity data for specific physical conditions. The user may then examine this data in as much detail as desired, from frequency-dependent opacities or multigroup opacities up to integrated Rosseland or Planck gray opacities. The data can be viewed and downloaded in tabular format or examined graphically.

The graphics code VIEWR, which was adapted from the T-2 Nuclear Data web page, takes the data from the TOPS code and displays it. The code can plot the data in 2 or 3 dimensions and allows the user broad choices in curve and background colors, curve types (line, dash, etc.) and grid options. Users can also limit the temperature, density, and photon energy ranges in order to study the opacities in greater detail.

Web Page Output:

The data base and support codes are accessed from the T-4 WWW home page at http://www.t4.lanl.gov. Two samples of the graphics output are presented to illustrate the range in detail that is available from the data base. Figure 1 presents the highest possible detail, showing individual line structures for aluminum. These data were used to compare to experimental transmission results from a German laser experiment. Figure 2 shows the integrated (over photon energy) opacities, which is the least detailed option. This plot is also an example of mixing data from two elements to make up an opacity table for a mixture. The structure in the plot arises from the atomic shell structure of carbon and iron as they are ionized.

Conclusions:

A limited version of the web page (with no graphics) has been operational for more than a year and has attracted over 600 users. The opacities have been used in astrophysical modeling and laboratory applications. The authors hope that the increased capabilities of the web page will attract new users both within the Laboratory and throughout the world.

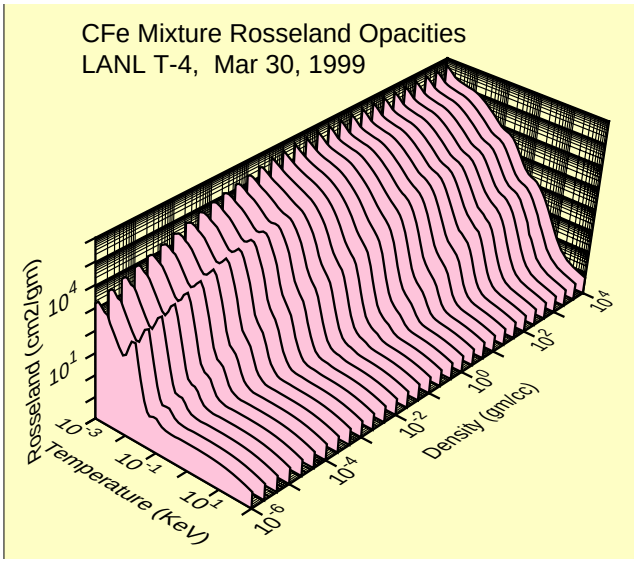

Figure 2: Plot of the integrated Rosseland opacities for a mixture of carbon and iron, covering the full temperature range of the data base and a normal SESAME density grid. Printed from the 3D gray opacity option.